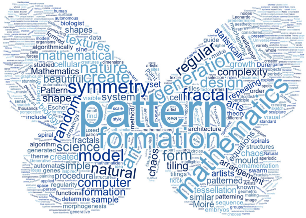
Advanced Mathematical Perspectives 1

Lecture 10: Diffusion and Difference Equations



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Fourier's analytical theory of heat (final form, 1822), devised in the Galileo-Newton tradition of controlled observation plus mathematics, is the ultimate source of much modern work in the theory of functions of a real variable and in the critical examination of the foundation of mathematics.

Eric Temple Bell, The Development of Mathematics (1940) p. 165

I fart in your general direction.

French soldier, Monty Python and the Holy Grail

Section 1

Diffusion Systems

Diffusion

- Assume mixing takes time, even in a gas
- Start with a concentration of some substance
- It spreads, or *diffuses* through the medium
- It's a model for
  - various fluids and gases
  - the spread of heat through a solid
  - some problems in electronics
  - spread of disease
- Key ideas
  - no material is created or destroyed, only moved around
  - rate of movement depends on concentrations themselves

Diffusion in 1D

Imagine a (thin) metal bar, being heated at one end

Assumptions

- Thin means we can approximate it as 1D
- *Conservation of energy* means the heat cannot be destroyed, so must just move around[1], so any change in temperature must be from inflow or outflow of heat.
- *Fourier's law:* the time rate of heat transfer through a material is proportional to the negative gradient in the temperature and to cross-sectional area.

[1] In reality, some heat is radiated away, but lets assume it isn't too much for the moment.

Diffusion in 1D

Constants and variables

- $u(x, t)$ is the temperature (in Kelvins)
  - at point $x \in [0, L]$ along the bar of length L
  - at time $t \geq 0$
- c = *specific heat*
  = amount of heat needed to increase a unit mass by one degree
- ρ = *density* (mass per unit length)
- k = *thermal conductivity*
- α = *thermal diffusivity*

$$\alpha = \frac{k}{c\rho}$$

i.e., how easy it is for heat to diffuse across the medium

material	α
copper	111
wood	0.082

Flow of heat

Fourier's law: the heat flux $q(x,t)$ is the amount of thermal energy that flows to the right per unit surface area per unit time, and is given by

$$q(x,t) = -k\frac{\partial u}{\partial x} \tag{1}$$

- intuitively, if there is a big temperature difference, heat flows faster
  - the minus sign is there because heat flows from hot to cold
- the RHS is a *partial* derivative
  - we don't teach you these until second year
  - think of it as the rate of change of heat along the bar
  - call this the gradient
  - if u is constant in time, then

$$\frac{\partial u}{\partial x} = \frac{du}{dx}$$

Conservation of energy

If no heat is added or lost[2] then any changes in temperature must result from flow of heat, so balancing these we get

$$\frac{\partial u}{\partial t} = -\frac{1}{c\rho}\frac{\partial q}{\partial x} \tag{2}$$

- LHS = change in temperature
- RHS = flow of heat divided by the amount needed to heat up region

[2] We can easily generalise, but let's keep it simple.

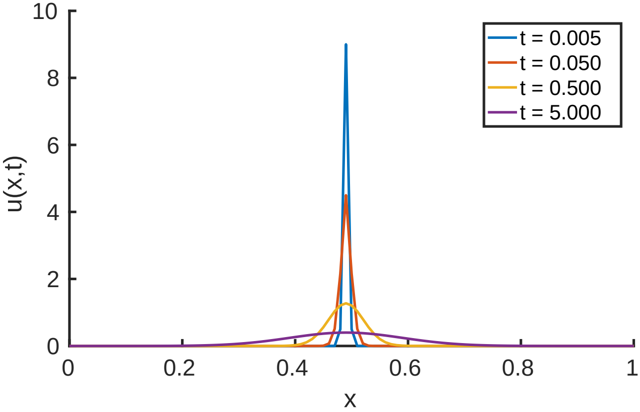
Rate of change

Substitute (1) into (2) and we get

$$\begin{aligned}\frac{\partial u}{\partial t} &= -\frac{1}{c\rho}\frac{\partial q}{\partial x} \\ &= \frac{k}{c\rho}\frac{\partial^2 u}{\partial x^2} \\ &= \alpha \nabla^2 u \qquad (3)\end{aligned}$$

- This is a PDE (a Partial Differential Equation), sometimes called the *heat equation*
- The operator ∇^2 is called Laplace's operator, or the *Laplacian*
- The solve it, we should add in initial an boundary conditions, but I am going to hack away

Example



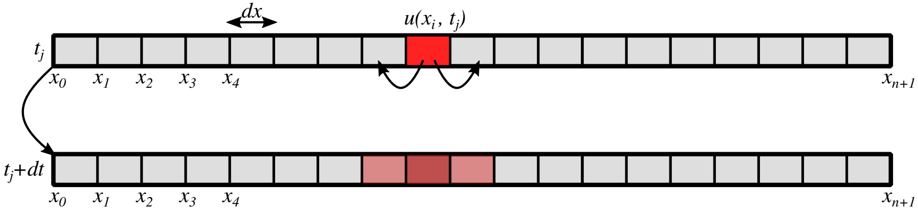
http://www.maths.adelaide.edu.au/matthew.roughan/notes/AMP1/files/diffusion1.gif

Diffusion as Smoothing

- We can think of diffusion as a “smoothing out” or spreading
  - notice the Gaussian (Bell curve) shape
- Underlying model is often Brownian motion of molecules
  - molecules bounce around at random, slowly diffusing outwards, or spreading kinetic energy (heat)
  - think of this as a “drunkard's walk”
  - more on this next week

Numerical Solution by Difference Equations

- I can't teach you how to solve these mathematically in one lesson (see extra notes at end of next lecture for a solution)
  - solution actually involves sinusoids and Fourier transforms
- But we can solve them numerically, by using an approximation called a difference equation (or a finite difference method)
- Intuitively, we break space and time into small pieces



Numerical Solution: time

The definition of derivative

$$\frac{dx}{dt} = \lim_{h \to 0} \frac{x(t+h) - x(t)}{h}$$

leads to an obvious approximation: *for small h*

$$\frac{dx}{dt} \simeq \frac{x(t+h) - x(t)}{h}$$

We'll use (without justifying) the same approximation for the partial derivative $\partial u / \partial t$ and rearrange (3) as follows

$$\begin{aligned} \frac{\partial u}{\partial t} &= \alpha \nabla^2 u \\ \frac{u(x, t+dt) - u(x,t)}{dt} &\simeq \alpha \nabla^2 u \\ u(x, t+dt) &\simeq u(x,t) + dt \times \alpha \nabla^2 u \end{aligned}$$

for small dt. We can iterate this, starting at $t = 0$, and calculating $u(\cdot, \cdot)$ forward in time, if we know the Laplacian.

Numerical Solution: Laplacian

Take a grid of points along our heated metal bar

$$x_i \quad = \quad i \times dx$$

for $i = 0, 1, 2, \ldots, n_x$ for small dx.

Approximate (as with time derivative)

$$\frac{\partial u}{\partial x} \simeq \frac{u(x_{i+1}, t) - u(x_i, t)}{x_{i+1} - x_i} = \frac{u(x_{i+1}, t) - u(x_i, t)}{dx}$$

Similarly we can approximate the second order partial derivative

$$\frac{\partial^2 u}{\partial x^2} \simeq \frac{u(x_{i+1}, t) - 2u(x_i, t) + u(x_{i-1}, t)}{dx^2}$$

Numerical Solution by Difference Equations

Put these together and we get

$$u(x_i, t_{j+1}) = u(x_i, t_j) + dt \times \alpha \left[\frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{dx^2} \right]$$

In MATLAB, given starting values of $u(0, x_j)$ we can write

```
for j = 1:num_t
   for i = 2:num_x-1
      u(i,j+1) = u(i,j) + ...
          alpha*dt*( u(i+1,j) - 2*u(i,j) + u(i-1,j) )/dx^2;
   end
end
```

We'll have a go with this in your practical.

Numerical Solution by Difference Equations

- Need to set initial and boundary conditions
- Need to set small enough *dt* and *dx* to make this work.
  - *e.g.*, stability requires $dt < dx^2/2\alpha$
- There are tricks involved in making this work well (*e.g.*, to make it efficient), or to rearrange it to be more stable, but if we don't mind a few extra compute cycles this will be OK for now.
- We can extend to 2D metal plate
  - we need 3D arrays $u(i, j, k)$

Activities

- Start by debugging some Matlab code to do diffusions
  - learn how to debug
  - see how I would code a function

Further reading I

Benoit Cushman-Roisin, *Environmental transport and fate: Diffusion equation*, https://thayer.dartmouth.edu/~d30345d/courses/engs43/DiffusionEquation.pdf.

Differential equations – notes, http://tutorial.math.lamar.edu/Classes/DE/TheHeatEquation.aspx.